Supplementary Information
Optical Properties of Prodigiosin and Obatoclax. Action Spectroscopy and Theoretical Calculations

Evangeline Drink,[a], Philippe Dugourd[a], Elise Dumont[b], Nils Aronssohn[b], Rodolphe Antoine[a,*], Claire Loison[a,*]

Received Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
First published on the web Xth XXXXXXXXXX 200X
DOI: 10.1039/b000000x

[a] *Institut Lumière Matière, UMR5306, Université Lyon 1-CNRS, Université de Lyon 69622 Villeurbanne cedex, France.* [b] *Laboratoire de Chimie, UMR5182, Ecole Normale Supérieure de Lyon, 69364 Lyon cedex 07, France.*
∗ *Corresponding authors. E-mail addresses: rodolphe.antoine@univ-lyon1.fr; claire.loison@univ-lyon1.fr*

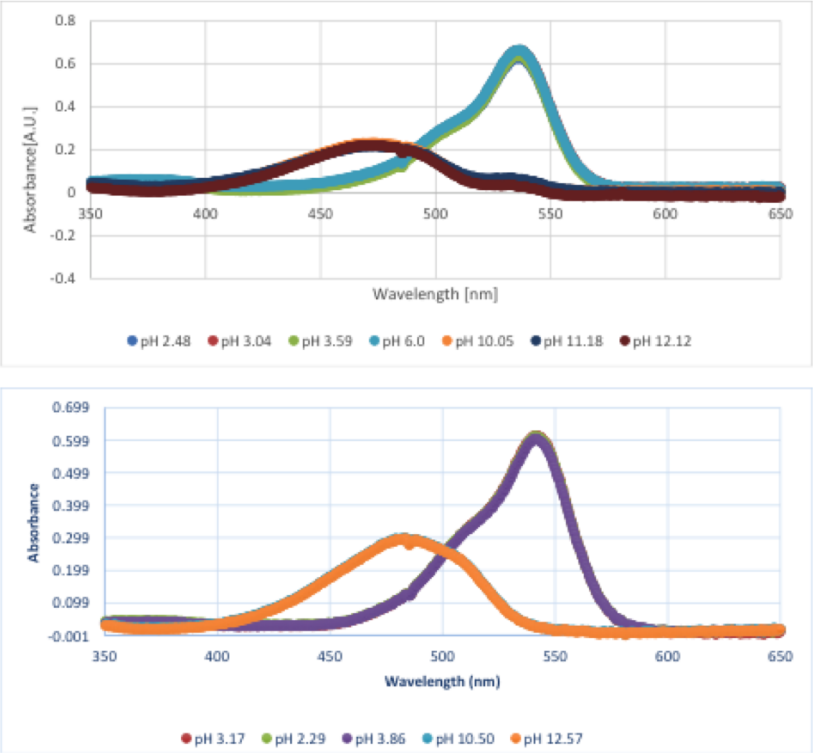

Fig. S1 Absorption Spectra of (top) prodigiosin, and (bottom) obatoclax in 1:1 Ethanol/Water Solution Under Various pH Conditions. Color online. pKa of PG-H^+/PG is 7.2 (Rizzo V. et al., J. Pharm. Sci., 88(1),73-78,1999), and pKa of OBX-H^+/PG is 7.9 (European Bioinformatics Institute's database). Please note that such values, obtained from spectrophotometric titrations, are macroscopic equilibrium acidity constants emerging from several concomitant titrations of different conformers in equilibrium. These conformers may have similar absorption spectra, but different pKa (see main Text, and Rizzo V. et al., J. Pharm. Sci., 88(1),73-78,1999).

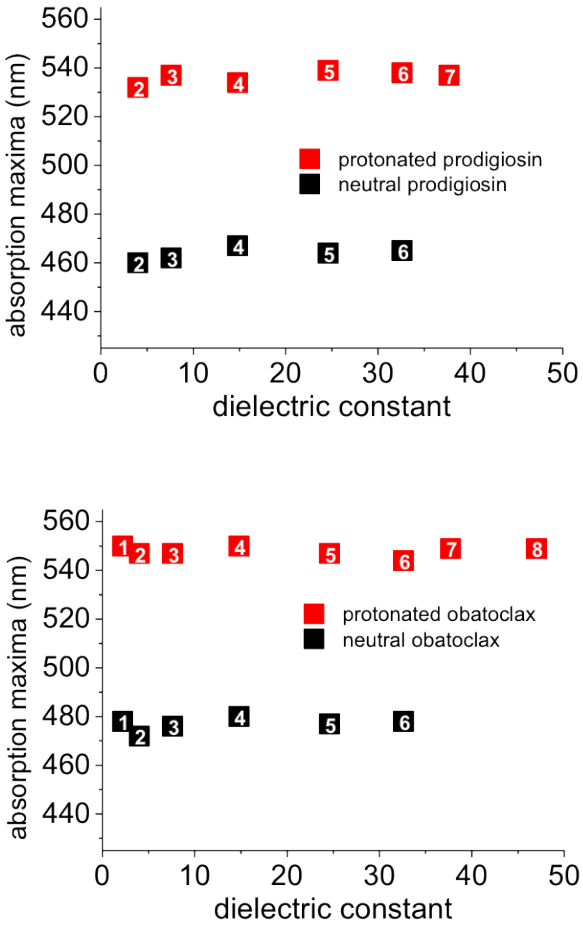

Fig. S2 Plots of absorption maxima in various solvents vs the dielectric constant for prodigiosin and obatoclax. (Dioxane, 1; Ether, 2;THF, 3; Pentanol, 4; Ethanol, 5; Methanol, 6; Ethylene Glycol, 7; DMSO, 8). Color online.

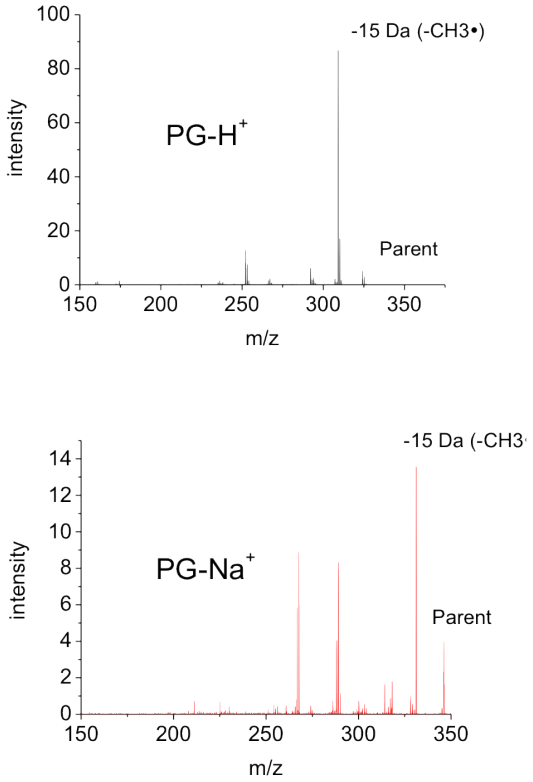

Fig. S3 Electrospray CID-MS2 spectra for (top) protonated prodigiosin PG-H^+ and (bottom) sodiated prodigiosin PG-Na^+ .

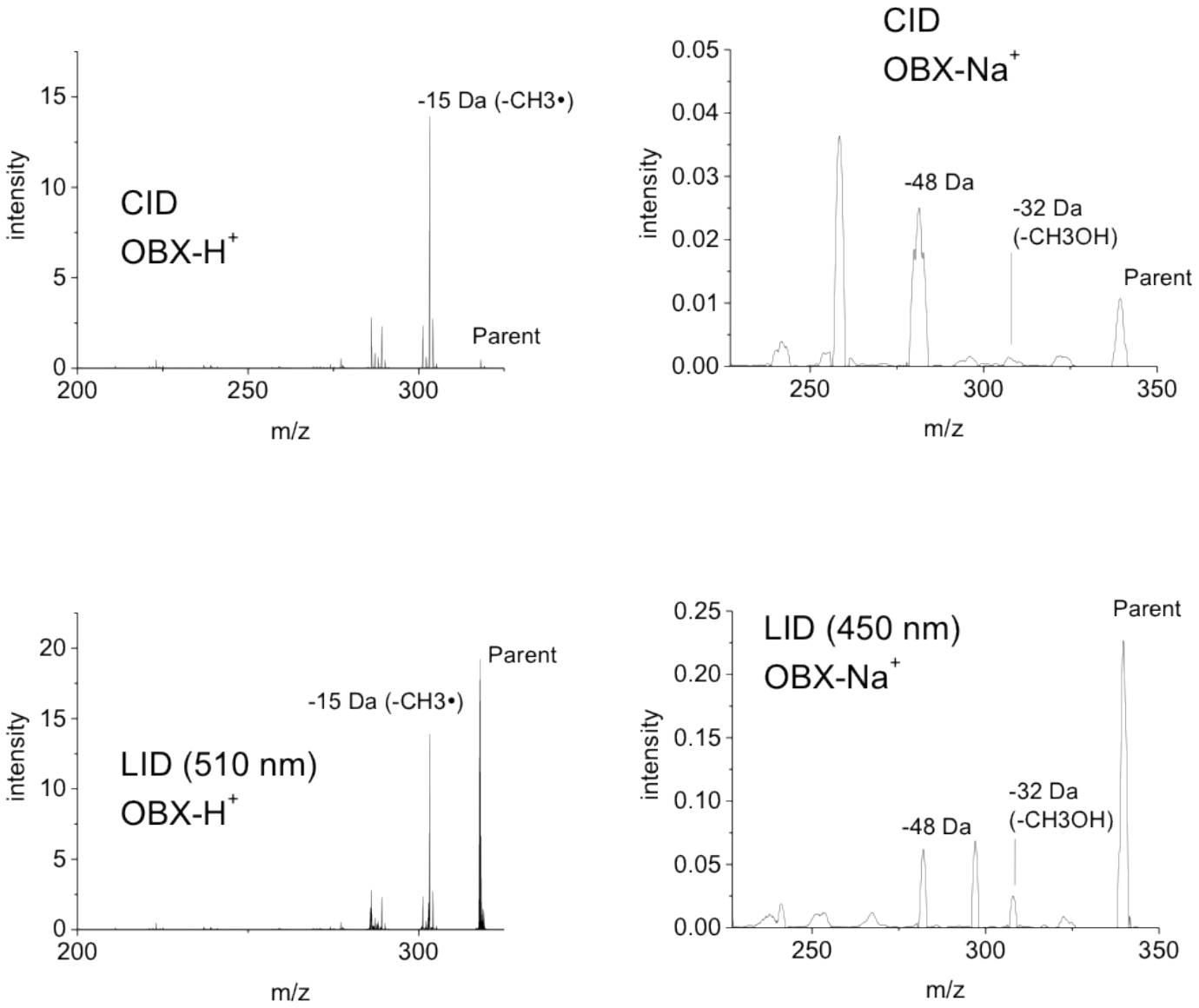

Fig. S4 Electrospray CID-MS2 and LID-MS2 spectra for (left) protonated obatoclax OBX-H^+ and (right) sodiated obatoclax OBX-Na^+.

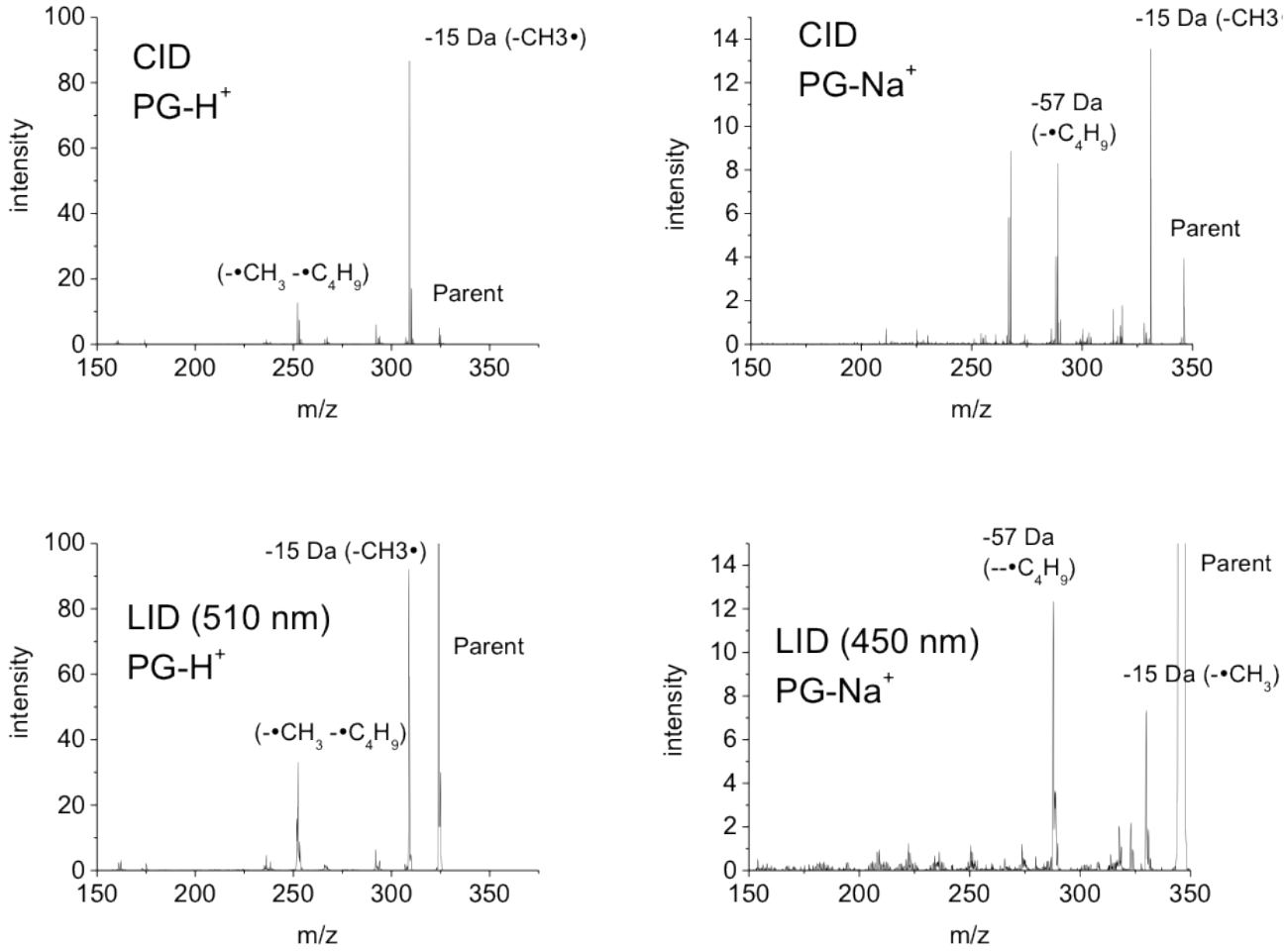

Fig. S5 Electrospray CID-MS2 and LID-MS2 spectra for (left) protonated prodigiosin PG-H^+ and (right) sodiated prodigiosin PG-Na^+.

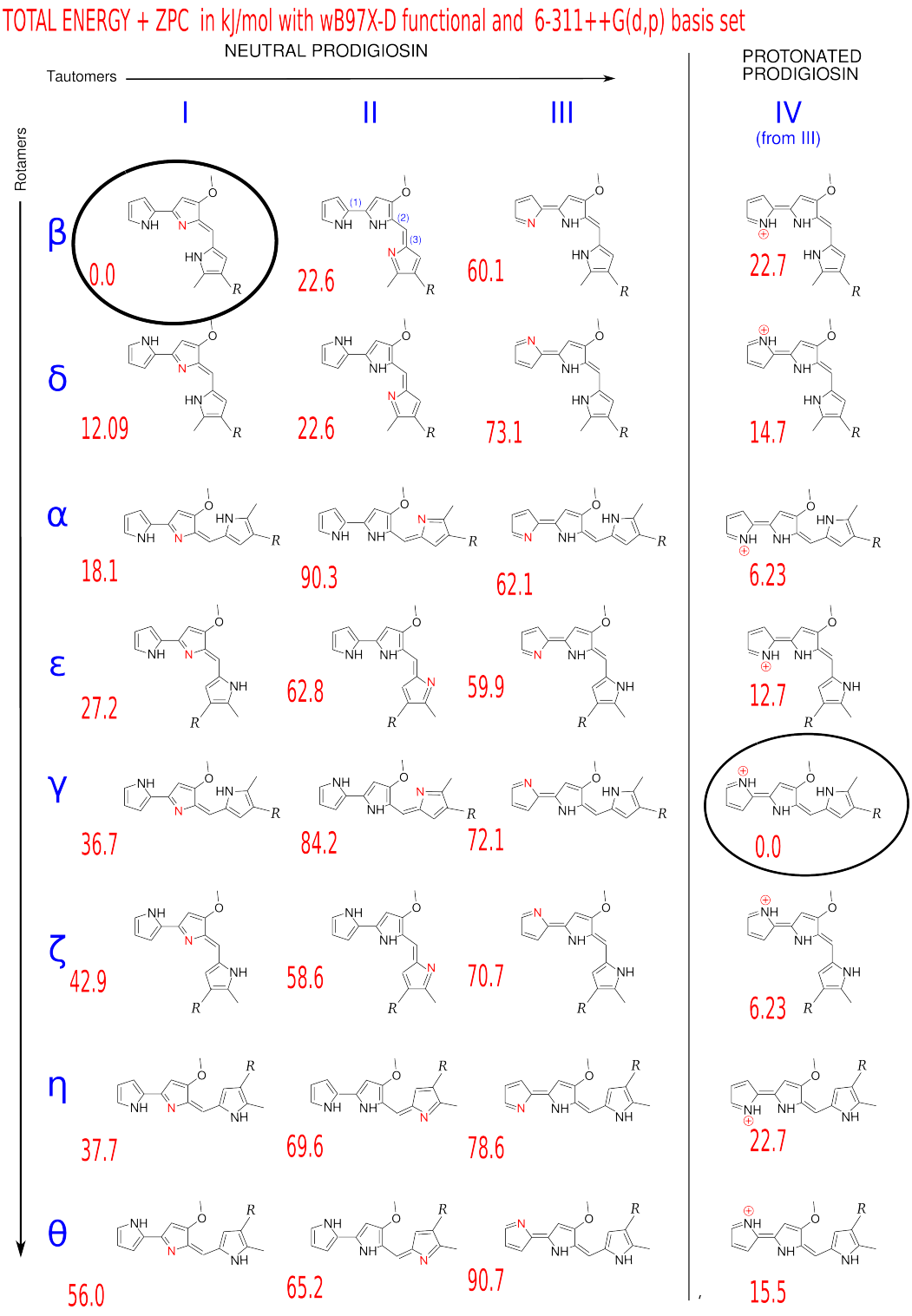

Fig. S6 Calculated total energies plus ZPC (6-311++G(d,p)/ωB97X-D) for the 32 conformers of our model Prodigiosin, neutral and protonated forms.

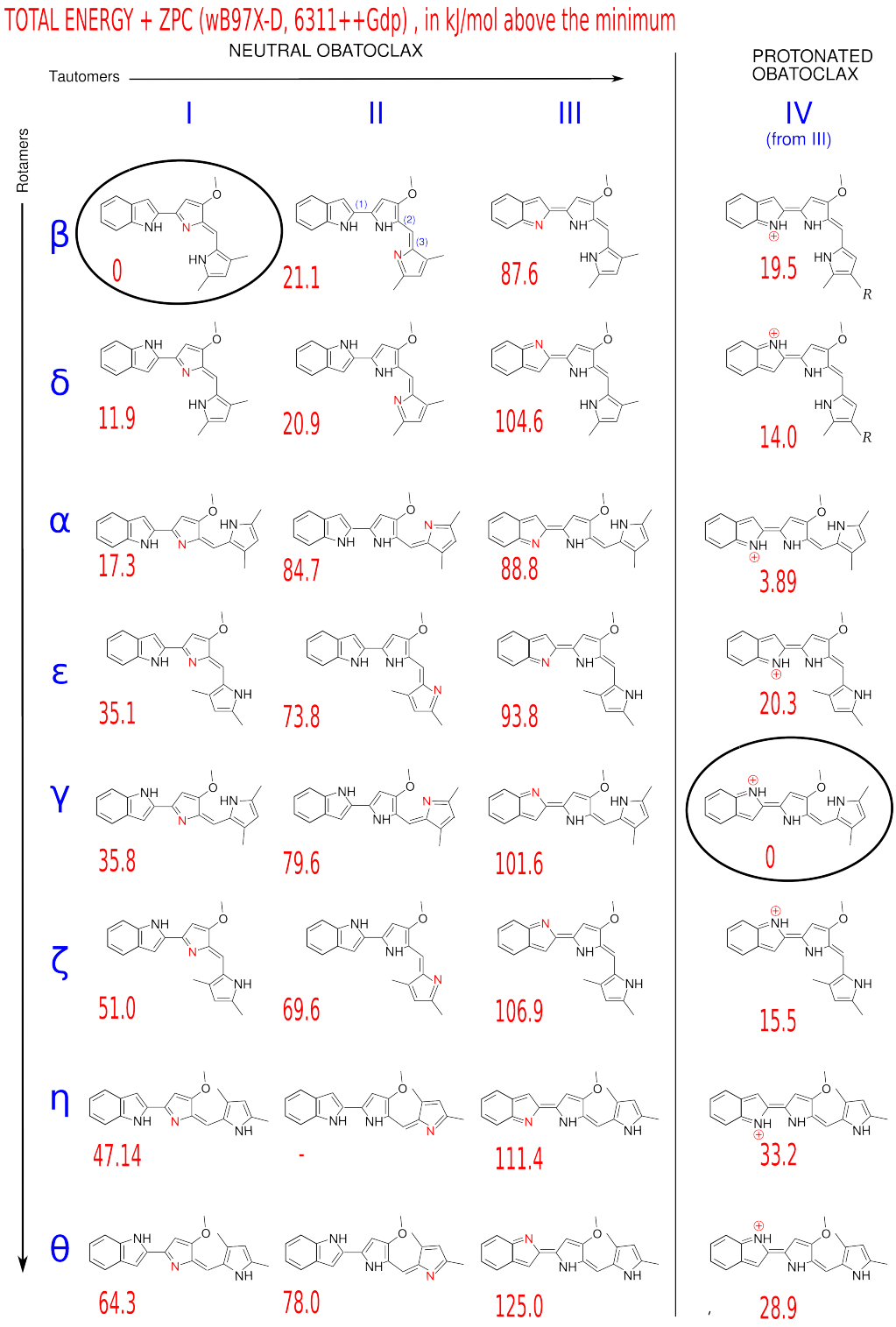

Fig. S7 Calculated total energies plus ZPC (6-311++G(d,p)/ωB97X-D) for the 32 conformers of Obatoclax, neutral and protonated forms.

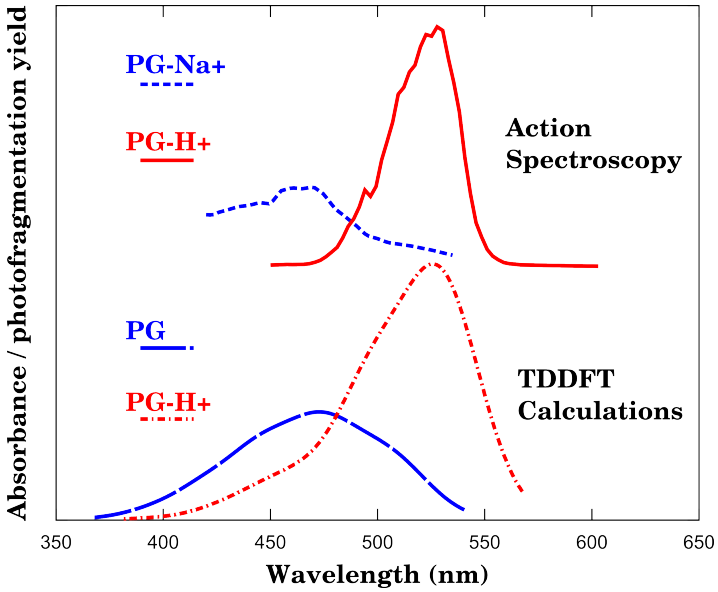

Fig. S8 Comparison of the gas-phase action spectra of protonated and sodiated prodigiosin, with the calculated absorption spectra of protonated and neutral prodigiosin. The action spectra have been vertically shifted to clarify the picture. Color online.